

METHODS FOR DETERMINING POLYPEPTIDE STRUCTURE, FUNCTION  
OR PHARMACOPHORE FROM COMPARISON OF POLYPEPTIDE SEQUENCES

ABSTRACT OF THE DISCLOSURE

The invention provides a method for separating  
5 two or more subsets of polypeptides within a set of  
polypeptides. The method includes the steps of: (a)  
determining a sequence comparison signature for each  
amino acid sequence in a set of amino acid sequences,  
wherein the sequence comparison signature includes  
10 pairwise comparison scores for the amino acid sequence  
compared to each of the other amino acid sequences in the  
set; (b) constructing a distance arrangement including  
the sequence comparison signatures related according to  
the distance between each of the sequence comparison  
15 signatures; and (c) identifying a first and second  
cluster of sequence comparison signatures in the distance  
arrangement, wherein the first cluster includes sequence  
comparison signatures for polypeptides having a similar  
protein fold or biological function, the protein fold or  
20 function being different compared to a protein fold or  
function of polypeptides having sequence comparison  
signatures in the second cluster.

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